Explorations – The Journal of Undergraduate Research, Scholarship and Creativity at Wright State

Volume 1
Issue 1 *Summer Undergraduate Research, Scholarship and Creative Activities Issue 2012*

Article 8

2012

Treatment of a Ring with Periodic Atomic Placement through Differential Geometry

Gregory Karjala
Wright State University, karjala.2@wright.edu

Lok Lew Yan Voon
Wright State University, lok.lewyanvoon@wright.edu

Treatment of a Ring with Periodic Atomic Placement through Differential Geometry

Gregory Karjala[1] and Lok Lew Yan Voon[2]

[1]Department of Physics, Wright State University, Dayton, Ohio 45435, USA

[2]College of Science and Mathematics, The Citadel, Charleston, South Carolina 29409, USA

Most treatments of Bloch's Theorem have relied on group theory or other mathematical methods for its proof. In this paper we give a derivation of the $\tilde{m}$ quantum number first proposed by Y.C Lee and Wei Z. Lee for the Benzene ring through the use of differential geometry. We also develop a Bloch style relationship relation for the benzene ring with an additional quantum number $\tilde{\alpha}$ .Through this treatment we show the usefulness of differential geometry in the theorist's toolkit when it comes to solid-state problems.

I. Introduction

Bloch's theorem is an important theorem in solid state physics. It treats a free electron in a periodic potential given by

$$U(r) = U(r + R) \qquad (1).$$

The most visible form of this theorem is given by

$$\psi(r + Na) = e^{ikNa}\psi(r) \qquad (2).$$

This theorem can be derived through the Nth-roots of unity by tying a string of periodic potentials into a circle.[1] Other derivations include the use of the translation group and Fourier Series.[1,2]In 2009 Y.C. Lee and Wei Z.Lee studied the rotational states of a Benzene ring. In their proof they treat a ring with a uniform distribution of particles. The ring is to be invariant under a rotation of $\frac{2\pi}{N}$, where N represents the number of particles. Due to symmetry considerations the wave function must respect the following relation

$$[\langle\varphi|\psi\rangle]^2 = \left[\left\langle\varphi + \tfrac{2\pi}{N}\middle|\psi\right\rangle\right]^2 \qquad (3).$$

In order to satisfy the above relation a phase factor of $e^{i\theta}$ is needed. This leads to

$$\left\langle\varphi + \tfrac{2\pi}{N}\middle|\psi\right\rangle = e^{i\theta}\langle\varphi|\psi\rangle \qquad (4).$$

Taking γ steps causes the phase difference to become accumulative leading to the following

$$\left\langle\varphi + \gamma\tfrac{2\pi}{N}\middle|\psi\right\rangle = e^{i\gamma\theta}\langle\varphi|\psi\rangle \qquad (5).$$

After an angular displacement, the phase difference the must be proportional to the displacement. Taking one angular step of $\frac{2\pi}{N}$ for example, and requiring it to be proportional to $\frac{2\pi}{N}$ we get the following equation

$$\left\langle\varphi + \frac{2\pi}{N}\middle|\psi\right\rangle = e^{i\tilde{m}\frac{2\pi}{N}}\langle\varphi|\psi\rangle \qquad \tilde{m} = 0, \pm1, \pm2, \pm3 \ldots\ldots \quad (6).$$

Were $\tilde{m}$ is the new quantum number the authors proposed, different from the angular momentum number m. This new quantum number plays the role of the wave number k used in a one dimensional crystal lattice.[3] With the advent of the carbon nano-tube

and other microscopic geometries the use of differential geometry can play an important role in this developing field.[4] The unifying theme of the textbook derivation of Bloch's Theorem through the use of the nth- roots and the Lee's derivation, is the use of a ring. This ring can be treated as an integral curve and we can apply the methods of differential geometry to it. In the next two sections we will, through geometric methods, give a second derivation of the quantum number $\tilde{m}$ and develop a Bloch style expression for the wave-function on a ring with an additional quantum number$\tilde{\alpha}$.

II. The p_z Orbital on a Cylindrical Surface.

The first step in our process was to find a mathematical technique that would predict a known physical property. The technique we choose was the Lie Derivative. The physical system we choose was a cylinder and the p_z orbital's that are normal to the cylindrical surface or in differential geometry terms the orbitals are parallel to each other. We take the circle integral curve of unit radius and use the polar plane for our work. The Lie Derivative describes the rate of change of a function, vector or tensor with respect to the tangent vector field of the integral curve. There is no unique parameterization of the unit circle. Two parameterizations of the tangent vector field of the integral curve for a circle do yield the polar basis vectors

$$V = \partial_r \qquad (7).$$

In this calculation we will use the p_z from the solution of the wave-function for hydrogen denoted below

$$\psi(\theta) = \sqrt{\frac{3}{8\pi}}\sin[\theta]^2 \qquad (8).$$

In an actual three dimensional atomic system these would represent p_y orbitals. Since we are working in the polar plane we will use these to represent the p_z orbitals. The next step is to take the Lie Derivative with respect to the radial basis.

$$\mathcal{L}_{V_2}\psi(\theta) = \partial_r\psi(\theta) = 0 \qquad (9).$$

This result implies that, with respect to the radial basis, that the orbitals are parallel at all angles between 0 and 2π. In vector calculus this statement would be read as the orbitals are normal to the surface of the cylinder.

III. Bloch Style relation, the $\tilde{m}$ quantum number, and the new quantum number $\tilde{\alpha}$.

Seeing the power of the Lie Derivative to make predictions, we now exploit a relation between the pullback of the flow of an integral curve and the Lie Derivative. This relation is given by

$$\Phi_t^* = e^{t\mathcal{L}_v} \qquad (10).$$

The t in the above expression represents the translation along the curve. The right hand side of the expression represents the exponential maps which takes a subset of the tangent space and maps it to the manifold. We will consider the ring integral curve with a uniform distribution of atomic positions separated by a distance of $\frac{2\pi}{N}$ were N represents the number of atoms. We will allow for an integral number of steps given by γ. Equation 11 now takes on the form

$$\Phi^*_{\frac{2\pi\gamma}{N}} = e^{\frac{2\pi\gamma}{N}\mathcal{L}_V} \quad N = 1,2,3 \ldots\ldots \quad \gamma = 0,1,2,3 \ldots\ldots \quad (11).$$

To generalize our equation we will consider a circle with arbitrary radius R so that our Lie Derivative in the argument of the exponent becomes

$$\mathcal{L}_V = R\partial_\theta \qquad (12).$$

We will now operate on the angular portion of the wave-function with the pullback of the flow

$$\Phi^*_{\frac{2\pi\gamma}{N}}\psi(\theta) = exp\left[\frac{2\pi\gamma}{N}R\partial_\theta\right]\psi(\theta) \qquad (13).$$

We can expand the right hand side out into a power series

$$\Phi^*_{\frac{2\pi\gamma}{N}}\psi(\theta) = \left(1 + \frac{2\pi\gamma}{N}R\partial_\theta + \frac{2\pi\gamma}{N}R\partial_\theta^2 \dots \dots\right)\psi(\theta) \qquad (14).$$

Equation 15 implies the pullback operator = $\psi\left(\theta + \frac{2\pi\gamma}{N}R\right)$

This means we can rewrite equation 15 into the following form given below

$$\psi\left(\theta + \frac{2\pi\gamma}{N}R\right) = exp\left[\frac{2\pi\gamma}{N}R\partial_\theta\right]\psi(\theta) \qquad (15).$$

This gives a translation relation along the ring.[5] Following along reference 2 we can regard gamma the quantum number $\tilde{m}$.

$$\psi\left(\theta + \frac{2\pi\tilde{m}}{N}R\right) = exp\left[\frac{2\pi\tilde{m}}{N}R\partial_\theta\right]\psi(\theta)$$

The next step is to impose the following periodic boundary condition

$$\psi\left(\theta + \frac{2\pi\tilde{m}}{N}R\right) = \psi(\theta) \qquad (16).$$

This condition requires the exponent equal one and hence complex. Now the ring has axial symmetry and gives us the linear equation.

$$L(\psi(\theta) = 0) \qquad (17).$$

Assuming equation 17 has a solution we can use the relation

$$\mathcal{L}_{\frac{\partial}{\partial\theta}} f = imf \qquad (18).$$

Using the scalar Lie derivative we have

$$\frac{\partial f}{\partial\theta} = imf \qquad (19).$$

If we assume the differential operator is equivalent to im , we can replace the angular basis in 15 with im. For clarity we will now denote m by $\tilde{\alpha}$. This leads us to the final form of the equation[6].

$$\psi\left(\theta + \frac{2\pi\tilde{m}}{N}R\right) = exp\left[\frac{2\pi\tilde{m}}{N}R\tilde{\alpha}\right]\psi(\theta) \quad \tilde{\alpha} = 0,1,2,3 \dots \dots \qquad (20).$$

Were we taking $\tilde{\alpha}$ to be the quantum number for the total angular momentum of the ring.

IV. Conclusion and Discussion

Using differential geometry we derived the $\tilde{m}$ quantum number proposed by Y.C Lee and Wei Lee. We derive a Bloch Style function with a quantum number $\tilde{\alpha}$. This is taken to be the total angular momentum of the ring. As a secondary result we show the usefulness of differential geometry in an application to Nano physics. New geometries can be studied theoretically for their properties through the use of differential geometry. These new geometries can then be grown in the laboratory. It is

hoped by the authors that differential geometry will be applied to other theorems of solid state physics.

Acknowledgments

We would both like to thank Dr. Morton Willatzen for his input on this project. Gregory Karjala would like to thank the Wright State Summer Undergraduate Research Program for enabling him to opportunity to conduct this research.

[1] Kittel, Charles. *Introduction to Solid State Physics*. New Delhi: Wiley Eastern, 1987. Print.

[2] Tung, Wu-Ki. *Group Theory in Physics*. Philadelphia: World Scientific, 1985. Print

[3] Lee, Y. C., and Wei Z. Lee. "Rotational States of a Benzene like Ring and Bloch's Theorem." *American Journal of Physics* 77.12 (2009): 1144. Print.

[4] Willatzen, Morten, and Lok C. Yoon. *Separable Boundary-value Problems in Physics*. Weinheim, Germany: Wiley-VCH Verlag, 2011. Print.

[5] Fecko, Marián. *Differential Geometry and Lie Groups for Physicists*. Cambridge: Cambridge UP, 2011. Print.

[6] Schutz, Bernard F. *Geometrical Methods of Mathematical Physics*. Cambridge: Cambridge UP, 1980. Print.